ENVIRONMENTAL MODELS AND SIMULATIONS

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Contents

Summary

The chapter presents the basic elements of modeling, how models can be applied for environmental management, a brief history of modeling, and a classification of models which can be used to understand the scientific basis for model development and application. A general validation and a validation of a prognosis based upon a relatively complex model are presented to illustrate the applicability of today's models in management.

The generality of relatively complex models is also discussed by use of the same model as a typical example. It is concluded that models have a certain but not full generality.

The most crucial problems in ecological modeling today are what can we do with a data base of poor quality? How can we achieve better parameter estimation? And how can we account for adaptation of species and shifts in species composition, which we do know take place in ecosystems? The field of ecological modeling has some suggestions to solve these problems which, in short, are making use of recently developed model types such as fuzzy models, new methods for parameter estimation, based on artificial intelligence and ecosystem theory and application of structurally dynamic models. The chapter in the last section discusses in which direction ecological modeling will move in the coming years and proposes the development of models integrating GIS and ecology,

a wider application for assessment of ecosystem health and environmental risks and integration of more ecosystem theory into our ecological models.

1. Introduction

Models are increasingly used in environmental management, because they are the only tool that is able to relate quantitatively the impact on an ecosystem with the consequences for the state of the ecosystem.

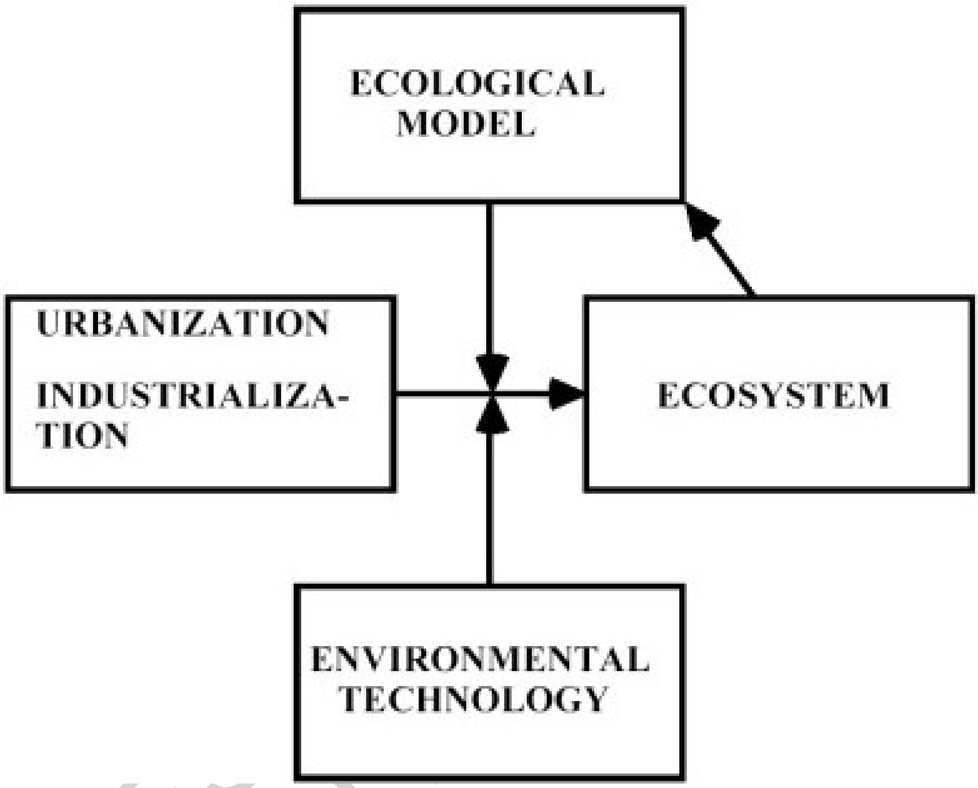

Figure 1: The figure illustrates the idea behind using models to find the relationship between the impact on ecosystems and the consequences in the ecosystems. The models can be used to select environmental technological solutions.

The idea behind the use of ecological management models is demonstrated in Figure 1. Urbanization and industrial development have had an increasing impact on the environment. Energy and pollutants are released into ecosystems, where they may cause more rapid growth of algae or bacteria, extinguish species, or alter the entire ecological structure. Now, an ecosystem is extremely complex, and so it is an overwhelming task to predict the environmental effects that such an emission will have. It is here that the model comes into the picture.

With sound ecological knowledge it is possible to extract the features of the ecosystem that are involved in the pollution problem under consideration, to form the basis of the ecological model. As indicated in Fig. 1, the model resulting can be used to select the environmental technology best suited for the solution of specific environmental problems, or legislation reducing or eliminating the emission set up. The figure represents the idea to introduce ecological modeling as a management tool round year 1970. Environmental management of today is more complex and must apply environmental technology, cleaner technology as an alternative to the present technology and ecological engineering or ecotechnology in combination with environmental legislation. The latter technology is applied to solve the problems of non-point or diffuse pollution, originating from agriculture and acidification. The importance of non-point pollution was hardly acknowledged before round 1975. Global environmental problems play furthermore a more important role today than twenty years ago. Abatements of the green house effect and depletion of the ozone layer are widely discussed and several international conferences on the governmental level have taken first steps toward the use of international standards to solve these crucial problems. Figure 2 attempts to illustrate the more complex picture of environmental management today.

Ecological models may be compared with geographical maps (which are models, too). Different types of maps serve different purposes. There are maps for airplanes, for ships, for cars, for railways, for geologists and archeologists and so on. They are all different, because they want to focus on different objects. They are also available in different scales according to the application of the map and to the underlying knowledge. Furthermore, a map contains never all details for a considered geographical area, because it would be irrelevant and disturb the main purpose of the map. If a map would contain all details for instance including the positions of all cars at a given moment, the map would be invalidated very rapidly, as cars would have moved to new positions. A map contains therefore only the knowledge that is relevant for the user of the map.

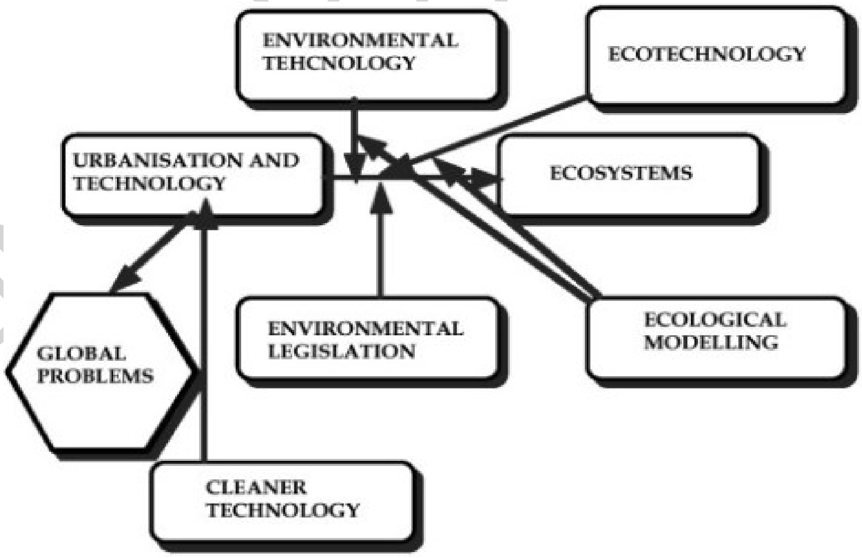

Figure 2: The idea behind the use of environmental models in environmental management. Environmental management of today is very complex and must apply environmental technology, alternative technology and ecological engineering or ecotechnology. In addition, the global environmental problems play an increasing role. Environmental models are used to select environmental technology, environmental legislation and ecological engineering.

An environmental model focuses in the same manner only on the objects of interest for the considered problem. It would disturb the main objectives of a model to include too many irrelevant details. There are many different ecological models of the same ecosystem, as the model edition is selected according to the model goals.

The field of ecological and environmental modeling has developed rapidly during the last two decades due essentially to three factors:

- the development of computer technology, which has enabled us to handle very complex mathematical systems.
- a general understanding of pollution problems, including that a complete elimination of pollution is not feasible ("zero discharge"), but that a proper pollution control with the limited economical resources available requires serious considerations of the influence of pollution impacts on ecosystems.
- our knowledge of environmental and ecological problems has increased significantly. We have particularly gained more knowledge about quantitative relations in ecosystems and between ecological properties and environmental factors.

2. Modeling Elements

In its mathematical formulation in environmental sciences, a model has five components:

1. **Forcing functions, or external variables,** which are functions or variables of an external nature that influence the state of the ecosystem. In a management context the problem to be solved can often be reformulated as follows: if certain forcing functions are varied, how will this influence the state of the ecosystem? The model is used to predict what will change in the ecosystem, when forcing functions are varied with time. The forcing functions under our control are often called **control functions.** The control functions in ecotoxicological models are for instance inputs of toxic substances to the ecosystems and in eutrophication models the control functions are inputs of nutrients. Other forcing functions of interest could be climatic variables, which influence biotic and abiotic components and the process rates. They are not controllable forcing functions.
2. **State variables** describe, as the name indicates, the state of the ecosystem. The selection of state variables is crucial to the model structure, but sometimes the choice is obvious. If, for instance, we want to model the bioaccumulation of a toxic substance, the state variables should be the organisms in the most important food chains and concentrations of the toxic substance in the organisms. In eutrophication models state variables will at least be the concentrations of nutrients and phytoplankton. When the model is used in a management context, the values of state variables predicted by changing the forcing functions can be considered as the results of the model, because the model will contain relations between the forcing functions and the state variables.
3. **Mathematical equations** are used to represent the biological, chemical and physical processes. They describe the relationship between the forcing functions and state variables, and between the state variables. The same type of process may be found in many different environmental contexts, which implies that the same equations can be

used in different models. This does not imply, however, that the same process is always formulated by use of the same equation. First, the considered process may be better described by another equation because of the influence of other factors. Second, the number of details needed or wanted to be included in the model may be different from case to case due to a difference in complexity of the system or/and the problem. Some modelers refer to description and mathematical formulation of processes as submodels. A comprehensive overview of submodels may be found in Jørgensen (1994) and Jørgensen et al. (1991).

4. **Parameters** are coefficients in the mathematical representation of processes. They may be considered constant for a specific ecosystem or part of an ecosystem. In causal models the parameter will have a scientific definition, e.g. the excretion rate of cadmium from a fish. Many parameters are not indicated in literature as constants but as ranges, but even that is of great value in the parameter estimation, as will be discussed further in the following text. In Jørgensen et al. (1991) a comprehensive collection of parameters in environmental sciences and ecology can be found. Our limited knowledge of parameters is one of the weakest points in modeling as will be touched on often throughout the chapter. Furthermore, the application of parameters as constants in our models is unrealistic due to the many feed-backs in real ecosystems. The flexibility of ecosystems is inconsistent with the application of constant parameters in the models. A new generation of models that attempts to use parameters varying according to some ecological principles seems a possible solution to the problem, but a further development in this direction is absolutely needed before we can achieve an improved modeling procedure reflecting the processes in real ecosystems. This issue is further discussed in Section 8.
5. **Universal constants,** such as the gas constant and atomic weights, are also used in most models.

Models can be defined as formal expressions of the relations between essential elements of a problem in mathematical terms. The first recognition of the problem is often verbal. This may be recognized as an essential preliminary step in the modeling procedure, which will be treated in more detail in the next section. The verbal model is, however, difficult to visualize and it is, therefore, more conveniently translated into a **conceptual diagram,** which contains the state variables, the forcing function and how these components are interrelated by mathematical formulations of processes.

Figure 3 illustrates a conceptual diagram of the nitrogen cycle in a lake. The state variables are nitrate, ammonium (which is toxic to fish in the unionized form of ammonia), nitrogen in phytoplankton, nitrogen in zooplankton, nitrogen in fish, nitrogen in sediment and nitrogen in detritus.

The forcing functions are: out- and inflows, concentrations of nitrogen components in the in- and outflows, solar radiation, and the temperature, which is not shown on the diagram, but that influences all the process rates. The arrows in the diagram illustrate the processes, and they are formulated by use of mathematical expressions.

Four significant steps in the modeling procedure should be defined in this section. They are verification, sensitivity analysis, calibration and validation:

Verification is a test of the *internal logic* of the model. Typical questions in the verification phase are: Does the model react as expected? Is the model stable in the long run? Does the model follow the law of mass conservation? Verification is largely a subjective assessment of the behavior of the model. To a large extent the verification will go on during the use of the model before the calibration phase, which has been mentioned above.

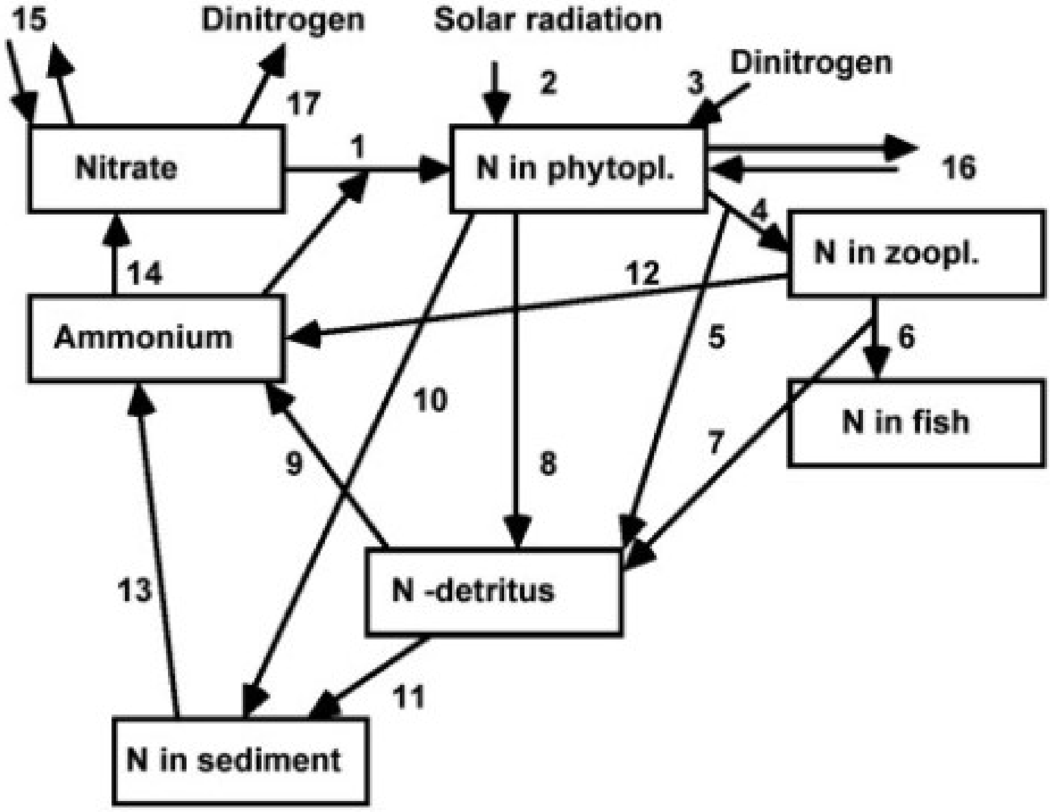

Figure 3: The conceptual diagram of a nitrogen cycle in an aquatic ecosystem. The processes are: 1) uptake of nitrate and ammonium by algae; 2) photosynthesis; 3) nitrogen fixation; 4) grazing with loss of undigested matter; 5), 6) and 7) are predation and loss of undigested matter; 8) mortality; 9) mineralization; 10) settling of algae; 11) settling of detritus; 12) excretion of ammonium from zooplankton; 13) release of nitrogen from the sediment; 14) nitrification; 15) and 16) are inputs/outputs; and 17) denitrification.

Sensitivity analysis follows verification. Through this analysis the modeler gets a good overview of the most *sensitive components of the model.* Thus, sensitivity analysis attempts to provide a measure of the sensitivity of either parameters, or forcing functions, or submodels to the state variables of greatest interest in the model. If a modeler wants to simulate a toxic substance concentration in, for instance, carnivorous insects as a result of the use of insecticides, he will obviously choose this state variable as the most important one, maybe in addition to the concentration of the toxic substance concentration in plants and herbivorous insects.

In practical modeling the sensitivity analysis is carried out by changing the parameters, the forcing functions or the submodels. The corresponding response on the selected state variables is observed. Thus, the sensitivity, S, of a parameter, P, is defined as follows:

$$S = [\Delta x/x]/[\Delta P/P], \quad (1)$$

where x is the state variable under consideration.

The relative change in the parameter value is chosen on the basis of our knowledge of the certainty of the parameters. If, for instance, the modeler estimates the uncertainty to be about 50%, he will probably choose a change in the parameters at ±10% and ±50% and record the corresponding change in the state variable(s). It is often necessary to find the sensitivity at two or more levels of parameter changes as the relation between a parameter and a state variable rarely is linear. A sensitivity analysis on submodels (process equations) can also be carried out. In this case a change in a state variable is recorded when the equation of a submodel is deleted from the model or changed to an alternative expression, for instance, with more details built into the submodel. Such results may be used to make structural changes in the model. If the sensitivity, for instance, shows that it is crucial for the model results to use a more detailed given submodel, this result should be used to change the model correspondingly. The selection of the complexity and the structure of the model should therefore work hand in hand with the sensitivity analysis.

A sensitivity analysis of forcing functions gives an impression of the importance of the various forcing functions and tells us which accuracy is required of the forcing function data.

Calibration is an attempt to find the best accordance between computed and observed data by variation of some selected parameters. It may be carried out by trial and error, or by use of software developed to find the parameters giving the best fit between observed and computed values. In some static models and in some simple models, which contain only a few well-defined, or directly measured, parameters, calibration may not be required.

Validation must be distinguished from verification. Validation consists of an objective test on how well the model outputs fit the data. The selection of possible objective tests will be dependent on the scope of the model, but the standard deviations between model predictions and observations and a comparison of observed and predicted minimum or maximum values of a particularly important state variable are frequently used. If several state variables are included in the validation, they may be given different weights.

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